Dimensional-scaling estimate of the energy of a large system from that of its building blocks: Hubbard model and Fermi liquid

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A simple, physically motivated, scaling hypothesis, which becomes exact in important limits, yields estimates for the ground-state energy of large, composed, systems in terms of the ground-state energy of its building blocks. The concept is illustrated for the electron liquid, and the Hubbard model. By means of this scaling argument the energy of the one-dimensional half-filled Hubbard model is estimated from that of a 2-site Hubbard dimer, obtaining quantitative agreement with the exact one-dimensional Bethe-Ansatz solution, and the energies of the two- and three-dimensional half-filled Hubbard models are estimated from the one-dimensional energy, recovering exact results for $U \to 0$ and $U \to \infty$ and coming close to Quantum Monte Carlo data for intermediate U.

Scaling techniques have propped up research since the early days of modern science. In the traditional version, which we call *discrete scaling*, one measures the properties of a body of diameter D to determine those of a similar body of diameter D', typically much larger than D. This approach is widely employed, e.g., in fluid dynamics. A more recent approach, extensively explored in the theory of critical phenomena, focuses on the relation between differential increments in the size L of a complex system and the resulting changes in its physical properties. To emphasize that L is a continuous variable, we refer to this procedure as *continuous scaling*. Continuous scaling finds a parallel in studies, also pioneered in the theory of critical phenomena, that treat the dimensionality d of a system as a continuous variable, and hence will be called *continuous dimensional scaling*. A classic illustration is the ϵ expansion, which extracts the properties of $(4 - \epsilon)$-dimensional systems from the exact mean-field solution of the 4-dimensional Gaussian model.[1] Other recent examples are found in dynamical mean-field theory[2] (DMFT) and in density-functional theory (DFT) for the Heisenberg model.[3]

Short as it is, this overview points to an as yet unprobed form of scaling: *discrete dimensional scaling*. We are unaware of attempts to extract the properties of a system of dimensionality d from the known properties of the same system in a different dimensionality. In the present work we explore this possibility. As a specific nontrivial model, to illustrate the general idea of discrete dimensional scaling, we choose the Hubbard model.

The Hubbard model was originally proposed on a three-dimensional lattice for the description of correlations in narrow-band materials.[4] Its two-dimensional version is often considered the correct minimal model for describing the cupper-oxide planes in cuprate superconductors.[5] The one-dimensional Hubbard model has received much attention due to the Luttinger liquid and Mott insulator phases it displays.[6] In the limit of infinite number of dimensions the Hubbard model was at the beginning of DMFT.[2] In all dimensions, the model serves as a laboratory and prime test case for our understanding of many-body physics and, in particular, strong Coulomb correlations. In standard notation and for any dimensionality d, the model reads

$$\hat{H} = \hat{T} + \hat{U} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow}, \quad (1)$$

where t and U are the kinetic energy and interaction parameters, respectively, and $\langle ij \rangle$ denotes a sum over nearest neighbors on a d-dimensional lattice.

The one-dimensional homogeneous Hubbard model has an exact solution in terms of the Bethe Ansatz,[6,7] one of the key results of which is a closed expression for the per-site ground-state energy at half filling, as a function of U,

$$\frac{E(U, d=1)}{t N_s} = -4 \int_0^\infty dx \frac{J_0(x) J_1(x)}{x[1 + \exp(Ux/2)]}, \quad (2)$$

where N_s is the number of sites and J_0 and J_1 are zero and first order Bessel functions. Such simple expressions for the total energy of nontrivial models are scarce in many-body physics, and where they exist they provide, in addition to considerable algebraic simplifications, insights into the nature of the model that would be hard to obtain from numerical data on its own.

The purpose of the present paper is to investigate to which extent knowledge aquired in low-dimensional situations, such as Eq. (2), can be useful in higher-dimensional systems, where exact solutions are not available. Mathematically, low and higher dimensional systems are solutions of the same type of differential equation, Schrödinger's equation. Physically, higher dimensional systems are built out of lower-dimensional building blocks. Both of these facts suggest that higher-dimensional systems cannot be arbitrarily different from

lower-dimensional ones. Mathematical and structural constraints imply the existence of (perhaps complicated) connections between quantities pertaining to one and to higher-dimensional systems. Here we identify and explore such constraints.

A first illustration of the concept of dimensional scaling is provided by bound homogeneous Coulomb systems, such as the Fermi liquid, described by the Hamiltonian

$$\hat{H}_{Clb} = -\frac{1}{2}\sum_i \nabla_i^2 + \sum_{i>j}\frac{1}{r_{ij}} + W, \qquad (3)$$

where W represents the constant potential energy of the uniform charge background, or of confining walls. For such a system satisfaction of the quantum-mechanical virial theorem[8] guarantees dynamical stability of the ground state. This theorem states that the total ground-state energy (comprising kinetic, potential and inter-action energy) is the negative of the kinetic energy, i.e.,[9] $E_{tot} = -E_{kin}$. Any relation of the form $E_{tot} = AE_{kin}$, with constant A, allows to write the identity $E_{tot}(d)/E_{tot}(d') = E_{kin}(d)/E_{kin}(d')$, which implies that the d-dimensional total energy can be obtained by scaling the d'-dimensional total energy according to

$$E_{tot}(d) = E_{kin}(d)\frac{E_{tot}(d')}{E_{kin}(d')}. \qquad (4)$$

Equation (4) is a first example of dimensional scaling, showing that the solution of a low-dimensional problem can generate a solution to a higher-dimensional problem of the same type. The virial theorem plays the role of the constraint mentioned above.

Next, we explore the question if similar expressions can also be obtained for the Hubbard model, whose total ground-state (GS) energy we denote by $E(U, d)$. Instead of the virial theorem, whose above form does not apply to the Hubbard model, we here base our analysis on the Hellman-Feynman theorem, which allows to cast the kinetic energy $E_{kin}(U, t) = E(U, t) - E_{int}(U, d)$ as

$$E_{kin}(U, t) = t\frac{\partial E(U, t)}{\partial t} = E(U, t) - U\frac{\partial E(U, t)}{\partial U}. \qquad (5)$$

The second term on the right-hand side vanishes both at small U, where the total ground-state energy $E(U, d)$ is linear in U, and at large U, where $E(U, d) \propto 1/U$. Hence, in both limits $E(U, d) = +E_{kin}(U, d)$. As for the electron liquid, this equality gives rise to the dimensional-scaling expression for the d-dimensional ground-state energy,

$$E(U, d) \approx E^{DS}(U, d) = E_{kin}(U, d)\frac{E(U, d')}{E_{kin}(U, d')} \qquad (6)$$

but unlike for the electron liquid, this is exact only in two limits, and approximate in between. Its use at all U embodies a linear dimensional-scaling hypothesis, whose validity must be carefully checked. Our first check is an application of Eq. (6) to one-dimensional Hubbard chains, whose energies we try to recover by means of

Eq. (6) from that of a zero-dimensional Hubbard model. A truly zero-dimensional model is useless for the present purpose, but a two-site system is as close to zero dimensionality as one can get without losing either of the two defining terms of the Hubbard model, the on-site inter-action and the nearest-neighbour hopping.

Applied to this case, Eq. (6) reads

$$E(U, 1) \approx E^{DS}(U, 1) = E_{kin}(U, 1)\frac{E(U, L = 2)}{E_{kin}(U, L = 2)}, \quad (7)$$

where L is the number of sites. $E(U, 1)$ is exactly known from Eq. (2), which thus allows a stringent test of the concept of dimensional scaling. The two-site Hubbard model can be diagonalized analytically for any U. For a half-filled band the exact per-site ground-state energy is

$$E(U, L = 2) = \frac{U}{4} - \sqrt{\frac{U^2}{16} + t^2}. \qquad (8)$$

The kinetic energies in Eq. (7) can be obtained from (2) and (8) via $E_{kin} = t\partial E/\partial t$. All ingredients on the right-hand side of (7) are thus known, and the resulting prediction for $E(U, 1)$ can be compared to the exact result for the infinite chain. This comparison, in Fig. 1, shows that linear dimensional scaling (dotted curve) almost coincides with the exact energy (dashed curve), illustrating that Eq. (7) with (8) is a near-exact representation of the true ground-state energy, even at intermediate U.

In more complicated cases the exact kinetic energies may not be known. We therefore also consider an approximation to Eq. (7) in which noninteracting kinetic energies are used in the scaling relation. For the dimer and the chain the noninteracting per-site kinetic energies are $E(U = 0, L = 2) = -t$ and $E(U = 0, d = 1) = -4t/\pi$, respectively. Hence, the noninteracting dimensional-scaling prediction for the per-site energy of the infinite chain is

$$E^{DS-0}(U, 1) = E(0, 1)\frac{E(U, L = 2)}{E(0, L = 2)} = \frac{U - \sqrt{U^2 + 16t^2}}{\pi}. \qquad (9)$$

We note that in the limits of very weak and very strong interactions this equation predicts $E^{DS}(U \to 0, 1) = -4t/\pi$ and $E^{DS}(U \to \infty, 1) = 0$, respectively. These are the same values also obtained from the Bethe-Ansatz expression (2), showing that in spite of the additional approximation entailed by using the noninteracting kinetic energy ratio instead of the interacting one, the dimensional scaling Ansatz is still exact for very weak and very strong interactions. For intermediate U, a numerical comparison between the exact Bethe-Ansatz result and the dimensional scaling estimate (9) is presented in Fig. 1 (full curve).

Figure 1 shows that, in spite of its simplicity, the dimensional scaling expression (7) reproduces the function $E(U, d = 1)$ almost exactly, while (9) provides a very reasonable approximation to it. Hence, the ground-state energy of the infinite chain is quantitatively recovered by
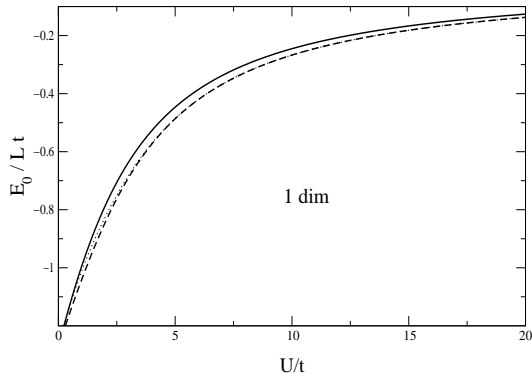
FIG. 1: Ground-state energy of the one-dimensional half-filled Hubbard model at positive U. Lower (dashed) curve: exact result, Eq. (2). Middle (dotted) curve: present expression (7), representing linear dimensional scaling with interacting kinetic energies. Upper (full) curve: present expression (9), representing linear dimensional scaling with noninteracting kinetic energies.
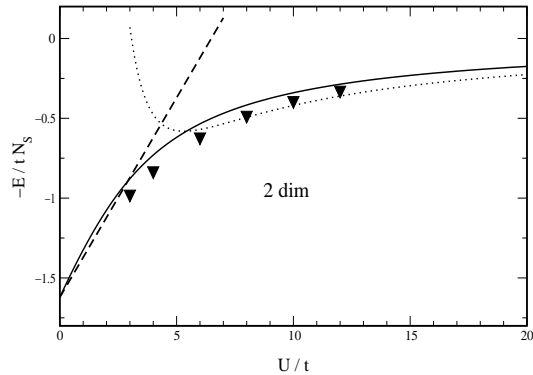

FIG. 2: Ground-state energy of the two-dimensional half-filled Hubbard model. Filled triangles: VMC data extrapolated to the thermodynamic limit, from Ref. 10. Dashed curve: Hartree-Fock energy. Dotted curve: $U \to \infty$ expansion of Ref. 16. Full curve: present expression (10).

suitable scaling of a simple dimer calculation. Crucially, this scaling involves an energy ratio, and not a length ratio.

After this exploration of the concept of dimensional scaling in situations in which the exact result is known in closed form, we now turn to a situation in which the higher-dimensional result is known only numerically. Namely, we attempt to predict the ground-state energy of the half-filled two-dimensional repulsive Hubbard model by applying virial-based dimensional scaling to the Lieb-Wu Bethe-Ansatz expression (2). This expression thus ceases to be our target to become the input on the right-hand side of Eq. (6).

The d-dimensional kinetic energy $E_{kin}(d)$ of the Hubbard model is already an in general unknown function of d, so that Eq. (6) cannot be used directly. We can, however, still employ noninteracting kinetic energies in the scaling factor. Equation (6) now reads

$$E(U,2) \approx E^{DS-0}(U,2) = E(0,2)\frac{E(U,1)}{E(0,1)}. \qquad (10)$$

Note that all quantities appearing on the right-hand-side of (10) are known: $E(U,1)$ is given by the Lieb-Wu formula (2), while $E(0,d)$ has the values[10,11,12] $E(0,1)/tN_s = -1.2732$, $E(0,2)/tN_s = -1.6211$, and $E(0,3)/tN_s = -2.0048$. As before, Eq. (10), which is by construction exact in $d = 1$ for any U, and at $U = 0$ in any d, is also already exact in any d in the limit $U \to \infty$: it follows from Eq. (2) that $E(U \to \infty, 1) = 0$, and hence $E^{LDS}(U \to \infty, d) = 0$, which is the correct $U \to \infty$ limit for the half-filled Hubbard model in any d. Dimensional scaling with noninteracting kinetic energies is thus still exact both for very weak and very strong correlations.

A more comprehensive check on (10) is obtained by comparing with precise numerical data obtained by Monte Carlo simulations.[10,12,13,14] Below we adopt as a benchmark the Variational Monte Carlo (VMC) data of Yokoyama and Shiba.[10] Their values do not deviate substantially from those obtained by other groups.[15] Figure 2 compares, for the $d = 2$ Hubbard model, the dimensional scaling expression (10) with these benchmark data, and with known large and small U limits.

Finally, we turn to the three-dimensional case. The 3d energies could be constructed in terms of the 2d ones, in the same way as before, but since the 2d energies themselves are not available in closed form this is not immediately practical. Instead, we subject the dimensional scaling idea to a more severe test, and try to predict the 3d energies directly from the 1d energies. Equation (6) then becomes

$$E(U,3) \approx E^{DS-0}(U,3) = E(0,3)\frac{E(U,1)}{E(0,1)}. \qquad (11)$$

A comparison of the resulting curve with QMC data and known large and small U limits is shown in Fig. 3.

Figures 2 and 3 show how 1d to 2d and 1d to 3d dimensional scaling, as expressed by Eqs. (10) and (11), merges into the exact expressions in the limits $U \to 0$ and $U \to \infty$, and comes close to the QMC data at intermediate U. Not unexpectedly, the step from $d = 1$ directly to $d = 3$ entails a larger margin of error than those from $d = 0$ to $d = 1$ and from $d = 1$ to $d = 2$, because the dimensional gap to be bridged by a simple scaling hypothesis is larger. The concatenation of the $d = 0$ to $d = 1$ expression with the $d = 1$ to $d = 3$ expression shows that an exact solution of the two-site system, followed by a double application of linear dimensional scaling, is sufficient to predict energies of the three-dimensional system
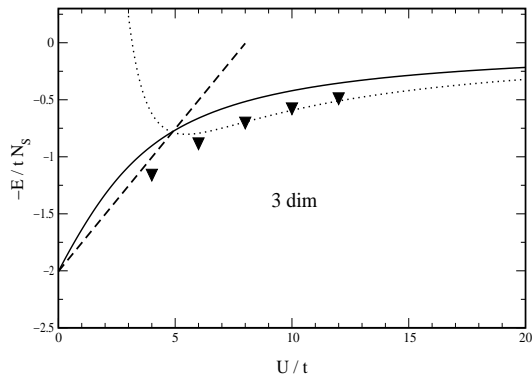
FIG. 3: Ground-state energy of the three-dimensional half-filled Hubbard model. Filled triangles: VMC data on a $6 \times 6 \times 6$ cluster (not extrapolated to the thermodynamic limit) from Ref. 10. Dashed curve: Hartree-Fock energy. Dotted curve: $U \to \infty$ expansion of Ref. 16. Full curve: present expression (6), representing linear dimensional scaling.

with a worst error of the order of 20 percent (and much less than that for most values of U), *without empirical adjustments or fitting parameters*. Remarkably, a two-site system thus contains enough nontrivial many-body effects that a simple scaling hypothesis is sufficient to recover from it a large part of the energy of chains, planes and bulk systems.

In summary, we have introduced the concept of dimensional scaling of ground-state energies. One explicit realization of this concept, based on the virial theorem, is exact for the electron liquids. Another, based on the Hellman-Feynman theorem, allows to predict the energies of an infinite Hubbard chain from that of a dimer with unexpected accuracy, and continues reasonable when extended to planes and bulk systems. Although the noninteracting kinetic energies in the scaling factor introduce an additional approximation, the dimensional scaling ansatz remains exact in the limits of weak and strong interactions.

These observations suggest the following questions for further investigation: (i) Does dimensional scaling also hold for other Hamiltonians? (ii) Is there a way to systematically improve on the dimensional scaling expression, reducing the remaining difference to the benchmark data without fitting or empirical input? (iii) Does dimensional scaling hold for other quantities than energies? A partial answer to question (i) is given by Eq. (4), which shows that dimensional scaling can also be expected for the electron liquids. A related, but not identical, type of dimensional scaling was recently also observed for the Heisenberg model.[3] Preliminary work on the negative U (attractive) Hubbard model also indicates the existence of simple scaling laws.[17] The present approach is expected to be particularly useful for model Hamiltonians that are not Bethe-Ansatz integrable, but can be solved in the 2-site limit, such as the periodic Anderson model. As for question (ii), the answer is 'yes'. A simple nonempirical way to improve on virial-based dimensional scaling will be presented in a forthcoming publication.[17]

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